6-heptyltetrahydro-2H-thiopyran-2-one

Inchi: InChI=1S/C12H22OS/c1-2-3-4-5-6-8-11-9-7-10-12(13)14-11/h11H,2-10H2,1H3
InchiKey: SYVWURCNFWCYOL-UHFFFAOYSA-N
Formula: C12H22OS
SMILES: CCCCCCCC1CCCC(=O)S1
Mol. weight [g/mol]: 214.37

Physical Properties

Property code	Value	Unit	Source
gf	-8.12	kJ/mol	Joback Method
hf	-329.13	kJ/mol	Joback Method
hfus	21.84	kJ/mol	Joback Method
hvap	52.79	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.159		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1789.00		NIST Webbook
ripol	2473.00		NIST Webbook
ripol	2473.00		NIST Webbook
tb	609.16	K	Joback Method
tc	826.54	K	Joback Method
tf	384.05	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.53	J/mol×K	609.16	Joback Method
cpg	510.37	J/mol×K	645.39	Joback Method
cpg	529.13	J/mol×K	681.62	Joback Method
cpg	546.81	J/mol×K	717.85	Joback Method
cpg	563.43	J/mol×K	754.08	Joback Method
cpg	579.00	J/mol×K	790.31	Joback Method
cpg	593.52	J/mol×K	826.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume